# Materials Computation Center, University of Illinois

Duane Johnson and Richard Martin, NSF DMR-9976550

*MCC Software Archive®*

## Research and Community Service

The MCC Software Archive was developed as a community service:
- to foster shared software resources,
- to reduce multiple code development,
- to encourage collaborations that leverage parallel code development efforts, and
- to support sharing of instructional codes, such as with MCC Summer School computational labs.

**Software posted at MCC is made available to (and from) the Computational Materials Community.**
The software is either be readily accessible or access is controlled by the author(s) of the software. Each software download requires a simple registration.

**Software presently includes codes involving**: Instructional, Analysis, DFT, Classical/Quantum Simulation, as well as links to other resources of which MCC is informed.

To contribute, please contact: **mcc@uiuc.edu**
Or see website for details: **www.mcc.uiuc.edu**

Materials Computation Center

**Software Archive**

**Example codes:**

**DataSpork – a MD/MC simulation analysis code that performs averaging, error and variance analysis, block averaging, correlation-time analysis, etc., using JAVA-based. DataSpork was developed for MatSE 385 at UIUC.**

**PARSEC – planewave pseudopotential (PW-PP) code for real-space electronic-structure calculations from J. Chelikowsky (Minnesota).**

**PETOT – DFT parallel PW DFT code from L. Wang (NERSC/LBL).**

**UPI – Path Integral MC code for Fermi and Bose systems from D. Ceperley (UIUC).**

**OHMMS – Object-oriented Multi-Scale Materials Simulator from J. Kim (MCC).**